

Zhichun Guo

Incoming Assistant Professor
Department of Computer Science
Emory University

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Research Interests

Graph Learning: enhance the effectiveness and efficiency of graph neural networks on various real-world applications

AI for Science: use AI models to deal with chemistry/biochemistry dilemmas in drug discovery

Trustworthy AI: enhance the fairness and explainability of AI models

Education

University of Notre Dame, Notre Dame, IN, US Aug 2019 – May 2024

Ph.D. in Computer Science and Engineering

Advisor: [Prof. Nitesh V. Chawla](#) (ACM & IEEE & AAAI & AAAS Fellow)

Committee members: [Dr. Wei Wang](#) (ACM Fellow), [Dr. Neil Shah](#), [Dr. Meng Jiang](#), [Dr. Xiangliang Zhang](#)

Fudan University, Shanghai, China Aug 2014 – Jul 2019

B.S. in Computer Science and Technology

Advisor: [Prof. Yang Chen](#)

Professional Experience

Incoming Assistant Professor Sep 2025 –
Computer Science, Emory University

Postdoctoral Researcher Jul 2024 – Present
Institute for Protein Design
Department of Biochemistry, University of Washington
Advisor: [Prof. David Baker](#)

Research Intern June 2023 – Sept 2023
Snap Inc.
Worked on efficient and effective link prediction
Mentors: Dr. Neil Shah and Dr. Tong Zhao

Research Intern June 2022 – Nov 2022
Snap Inc.
Worked on accelerating link prediction for inference
Mentors: Dr. Neil Shah and Dr. Tong Zhao

Research Assistant April 2018 – Aug 2018
University of Notre Dame
Worked on interactive visualization to evaluate scholarly performance
Advisor: [Prof. Chaoli Wang](#)

Research Assistant Jul 2017 – Sep 2017
Chinese Academy of Sciences
Worked on visual analysis of human mobility in cities
Advisor: [Prof. Lei Shi](#)

Honors and Awards

Snap Research Fellowship	2022
IEEE VIS Inclusivity & Diversity Scholarship	2022
Hui-Chun Chin and Tsung-Dao Lee Chinese Undergrad Research Endowment	2017
First Prize Scholarship for Outstanding Students	2017
EMC Scholarship for Outstanding Students	2016
NSF Center for Computer Assisted Synthesis Travel Award	2023
IJCAI Travel Grant	2023
SDM Student Travel Award	2023

Publications [Google Scholar]

20 peer-reviewed research papers published in ICML, ICLR, NeurIPS, AAAI, WWW, IJCAI, etc.

Citations: 810+, **h-index:** 15, **i10-index:** 19

Selected Peer-Reviewed Publications

- [ICML'23] **Linkless Link Prediction via Relational Distillation**
Zhichun Guo, William Shiao, Shichang Zhang, Yozen Liu, Nitesh V. Chawla, Neil Shah, Tong Zhao
International Conference on Machine Learning, 2023
- [IJCAI'23] **Graph-based Molecular Representation Learning**
Zhichun Guo, Kehan Guo, Bozhao Nan, Yijun Tian, Roshni G. Iyer, Yihong Ma, Olaf Wiest, Xiangliang Zhang, Wei Wang, Chuxu Zhang, Nitesh V. Chawla
International Joint Conference on Artificial Intelligence Survey Track, 2023
- [AAAI'23] **Boosting Graph Neural Networks via Adaptive Knowledge Distillation**
Zhichun Guo, Chunhui Zhang, Yujie Fan, Yijun Tian, Chuxu Zhang, Nitesh V. Chawla
AAAI Conference on Artificial Intelligence, 2023
- [TVCG'22] **SD²: Slicing and Dicing Scholarly Data for Interactive Evaluation of Academic Performance**
Zhichun Guo, Jun Tao, Siming Chen, Nitesh V. Chawla, Chaoli Wang
IEEE Transactions on Visualization and Computer Graphics, IF:5.23, 2022
- [WWW'21] **Few-Shot Graph Learning for Molecular Property Prediction**
Zhichun Guo, Chuxu Zhang, Wenhao Yu, John Herr, Olaf Wiest, Meng Jiang, Nitesh V. Chawla
The Web Conference, 2021
- [CIKM'20] **GraSeq: Graph and Sequence Fusion Learning for Molecular Property Prediction**
Zhichun Guo, Wenhao Yu, Chuxu Zhang, Meng Jiang, Nitesh V. Chawla
ACM International Conference on Information and Knowledge Management, 2020
- [NeurIPS'24] **Pure Message Passing Can Estimate Common Neighbor for Link Prediction**
Kaiwen Dong, **Zhichun Guo**, Nitesh V. Chawla
Conference on Neural Information Processing Systems, 2024
- [NeurIPS'24] **Test-time Aggregation for Collaborative Filtering**
Mingxuan Ju, William Shiao, **Zhichun Guo**, Yanfang Ye, Yozen Liu, Neil Shah, Tong Zhao
Conference on Neural Information Processing Systems, 2024
- [NeurIPS'24] **Can LLMs Solve Molecule Puzzles? A Multimodal Benchmark for Molecular Structure Elucidation**
Kehan Guo, Bozhao Nan, Yujun Zhou, Taicheng Guo, **Zhichun Guo**, Mihir Surve, Zhenwen Liang, Nitesh V Chawla, Olaf Wiest, Xiangliang Zhang
Conference on Neural Information Processing Systems Datasets and Benchmarks Track, 2024
- [NeurIPS'23] **What Indeed Can GPT Models Do in Chemistry? A Comprehensive Benchmark on Eight Tasks**
Taicheng Guo, Kehan Guo, Bozhao Nan, Zhenwen Liang, **Zhichun Guo**, Nitesh V. Chawla, Olaf Wiest, Xiangliang Zhang
Conference on Neural Information Processing Systems Datasets and Benchmarks Track, 2023
- [ICLR'23] **Link Prediction with Non-Contrastive Learning**
William Shiao, **Zhichun Guo**, Tong Zhao, Evangelos E. Papalexakis, Yozen Liu, Neil Shah
International Conference on Learning Representations, 2023
- [ICLR'23] **Learning MLPs on Graphs: A Unified View of Effectiveness, Robustness, and Efficiency**
Yijun Tian, Chuxu Zhang, **Zhichun Guo**, Xiangliang Zhang, Nitesh V. Chawla
International Conference on Learning Representations, 2023
[Spotlight Paper]
- [EACL'23] **A Survey of Multi-task Learning in Natural language Processing: Regarding Task Relatedness and Training Methods**
Zhihan Zhang, Wenhao Yu, Mengxia Yu, **Zhichun Guo**, Meng Jiang
Conference of the European Chapter of the Association for Computational Linguistics, 2023

- [Chem. Sci'23] **On the Use of Real-World Datasets for Reaction Yield Prediction**
Mandana Saebi, Bozhao Nan, John Herr, Jessica Wahlers, **Zhichun Guo**, Andrzej Zurański, Thierry Kogej, Per-Ola Norrby, Abigail Doyle, Olaf Wiest, Nitesh V. Chawla
Chemical Science, *IF:9.97*, 2023
- [LoG'22] **FakeEdge: Alleviate Dataset Shift in Link Prediction**
Kaiwen Dong, Yijun Tian, **Zhichun Guo**, Yang Yang, Nitesh V. Chawla
Learning on Graphs Conference, 2022
- [LoG'22] **Flashlight: Scalable Link Prediction with Effective Decoders**
Yiwei Wang, Bryan Hooi, Yozen Liu, Tong Zhao, **Zhichun Guo**, Neil Shah
Learning on Graphs Conference, 2022
- [IJCAI'22] **RecipeRec: a heterogeneous graph learning model for recipe recommendation**
Yijun Tian, Chuxu Zhang, **Zhichun Guo**, Chao Huang, Ronald Metoyer, Nitesh V. Chawla
International Joint Conference on Artificial Intelligence, 2022
- [IJCAI'22] **Recipe2Vec: Multi-model Recipe Representation Learning with Graph Neural Networks**
Yijun Tian, Chuxu Zhang, **Zhichun Guo**, Yihong Ma, Ronald Metoyer, Nitesh V. Chawla
International Joint Conference on Artificial Intelligence, 2022
- [CIKM'22] **Hierarchical spatio-temporal graph neural networks for pandemic forecasting**
Yihong Ma, Patrick Gerard, Yijun Tian, **Zhichun Guo**, Nitesh V. Chawla
ACM International Conference on Information and Knowledge Management, 2022
- [EMNLP'21] **Sentence-Permuted Paragraph Generation**
Wenhao Yu, Chenguang Zhu, Tong Zhao, **Zhichun Guo**, Meng Jiang
Conference on Empirical Methods in Natural Language Processing, 2021
- [CIKM'21] **Action Sequence Augmentation for Early Graph-based Anomaly Detection**
Tong Zhao, Bo Ni, Wenhao Yu, **Zhichun Guo**, Neil Shah, Meng Jiang
ACM International Conference on Information and Knowledge Management, 2021
- [HCIS'21] **Visual Analysis of Steady-State Human Mobility in Cities**
Lei Shi, **Zhichun Guo**, Tao Jiang, Ruiyu Fang, Yang Chen, Ye Zhao, Xiatian Zhang, Min Dai
Human-centric Computing and Information Sciences, *IF:6.60*, 2021
- [WWWJ'19] **Exploring the power of social hub services**
Qingyuan Gong, Yang Chen, Xiaolong Yu, Chao Xu, **Zhichun Guo**, Yu Xiao, Fehmi Ben Abdesslem, Xin Wang, Pan Hui
World Wide Web, 2019

Preprints and Under Submissions

- [ICLR'25] **Node Duplication Improves Cold-start Link Prediction**
Zhichun Guo, Tong Zhao, Yozen Liu, Kaiwen Dong, William Shiao, Neil Shah, Nitesh V. Chawla
Under Submission, 2024

Talks and Presentations

Invited Talks

Department of Computer Science, Emory University	Mar 2024
Department of Computer Science and Engineering, Michigan State University	Mar 2024
Department of Computer Science, UT Dallas	Feb 2024
Department of Computer Science, Virginia Tech	Feb 2024
Department of Computer Science, University of Houston	Feb 2024
Department of Computer Science, Florida State University	Feb 2024
Learning on Graphs Seminar	Aug 2023

Conference & Forum Presentations

Graph-based Molecular Representation Learning	IJCAI , Conference Presentation, 2023
Linkless Link Prediction via Relational Distillation	ICML , Conference Presentation, 2023
Generalizing GNNs for Multi-applications with Effective Training Strategies	SDM , Doctoral Forum Presentation, 2023
Boosting Graph Neural Networks via Adaptive Knowledge Distillation	AAAI , Conference Presentation, 2023
Slicing and Dicing Scholarly Data for Interactive Evaluation of Academic Performance	VIS , Conference Presentation, 2022
Few-Shot Graph Learning for Molecular Property Prediction	WWW , Conference Presentation, 2021
GraSeq: Graph and Sequence Fusion Learning for Molecular Property Prediction	CIKM , Conference Presentation, 2020

Teaching Experience

NSF Center for Computer Assisted Synthesis Training Videos 2021

- Role: Lecturer
- Lectures (received 5.6k+ views):
 - Representing Molecules as Graphs for Graph Neural Networks
 - Training Graph Neural Networks for Reaction Prediction
 - Deep Learning Based Molecular Representation Learning
 - Transfer Learning, Meta-Learning, and Meta-Transfer Learning
 - String-based Representation of Molecules: SMILES, SMARTS and SELFIES

CSE 20312 Data Structures (Undergraduate Level) Spring 2020

- Role: Teaching Assistant
- Duties: Review assignments, Q&A during office hours, Grade

Professional Services

Organizer

PC for KDD'24 Lecture-style Tutorials 2024
Learning on Graphs Conference (**LoG**) Meetup 2023

Conference PC/Reviewer

International Conference on Learning Representations (**ICLR**) 2024
AAAI Conference on Artificial Intelligence (**AAAI**) 2025, 2024, 2023
SIAM International Conference on Data Mining (**SDM**) 2024
Learning on Graphs Conference (**LoG**) 2023
Neural Information Processing Systems (**NeurIPS**) 2024, 2023
SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD**) 2024, 2023, 2022
International Joint Conference on Artificial Intelligence (**IJCAI**) 2024, 2023
Conference on Information and Knowledge Management (**CIKM**) 2024
IEEE International Conference on Data Mining (**ICDM**) 2022
IEEE Visualization Conference (**VIS**) 2021

Journal Invited Reviewer

IEEE Transactions on Pattern Analysis and Machine Intelligence (**TPAMI**) 2024
IEEE Transactions on Knowledge and Data Engineering (**TKDE**) 2024, 2023
ACM Transactions on Knowledge Discovery from Data (**TKDD**) 2024, 2023, 2022
IEEE Transactions on Big Data 2023
Digital Discovery 2023
IEEE Transactions on Neural Networks and Learning System (**TNNLS**) 2024, 2023, 2022
Data Mining and Knowledge Discovery (**DAMI**) 2023, 2022
Bioinformatics 2022
Neurocomputing 2023, 2022
Visual Informatics 2023, 2022
Journal of Social Computing 2022
Journal of Big Data 2022, 2021
Journal of Artificial Intelligence Research 2021

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